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Grassmann integral and Balian–Brézin decomposition in Hartree–Fock–Bogoliubov matrix elements

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ABSTRACT

We present a new formula to calculate matrix elements of a general unitary operator with respect to Hartree–Fock–Bogoliubov states allowing multiple quasi-particle excitations. The Balian–Brézin decomposition of the unitary operator [R. Balian, E. Brézin, Il Nuovo Cimento B 64 (1969) 37] is employed in the derivation. We found that this decomposition is extremely suitable for an application of Fermion coherent state and Grassmann integrals in the quasi-particle basis. The resultant formula is compactly expressed in terms of the Pfaffian, and shows the similar bipartite structure to the formula that we have previously derived in the bare-particles basis [T. Mizusaki, M. Oi, Phys. Lett. B 715 (2012) 219].

1. Introduction

In nuclear many-body physics, evaluations of matrix elements of many-body operators have been a major obstacle to implementations of sophisticated methods and theories beyond the mean-field approximation. Nuclear physicists have put effort into finding convenient formulae [1–3] to calculate matrix elements (and overlaps) with respect to Hartree–Fock–Bogoliubov (HFB) states. But difficulties remained in the obtained formulae. Although there were some numerical attempts to circumvent difficulties associated with the known formulae [4,5], there had not been any significant progress for decades in an analytical attempt to make a breakthrough. Recently such a breakthrough was achieved by Robledo who was successful in deriving a new formula in terms of the Pfaffian [6] with Fermion coherent states and Grassmann integral [7]. After his pioneering work, many studies followed by exploiting these mathematical tools in the HFB matrix elements [8–11].

The latest focus in this research field is to find a formula to evaluate HFB matrix elements with multiple quasi-particle excitations [9–11] $\langle\phi'|c_{\nu'_1}\cdots c_{\nu'_{n'}}c^\dagger_{\nu_1}\cdots c^\dagger_{\nu_n}|\phi\rangle$, where $|\phi\rangle$ and $|\phi'\rangle$ are different HFB states. The creation and annihilation operators for bare particles are denoted by $c^\dagger$ and c respectively, hence $c_\nu|0\rangle = 0$. $|0\rangle$ stands for the true vacuum. These matrix elements have been evaluated conventionally by the generalized Wick's theorem. Recently, alternative approaches [9–11] were obtained by means of Fermion coherent states and Grassmann integral. The resultant formulae are expressed in terms of the Pfaffian, which can describe the matrix elements in a more compact manner than those obtained by the generalized Wick's theorem. The new formulae overcome a combinatorial complexity associated with practical applications of the generalized Wick's theorem. (It is worth mentioning that there was an attempt to derive a compact formula before the publication of Robledo's Pfaffian formula. Ref. [12] adapts Gaudin's theorem in the finite-temperature formalism so as to derive an equivalent formula, but it is not expressed in terms of the Pfaffian.)

In this Letter, we would like to present another formula that evaluates matrix elements of a unitary operator sandwiched by arbitrary HFB states with multiple quasi-particle excitations,

$$\langle\phi|a_{\nu'_1}\cdots a_{\nu'_{n'}}[\theta]a^\dagger_{\nu_1}\cdots a^\dagger_{\nu_n}|\phi\rangle. \tag{1}$$

The quasi-particle basis $(a, a^\dagger)$ is obtained through a canonical transformation (called the Bogoliubov transformation) of the bare-particle basis $(c, c^\dagger)$,

$$a^\dagger_\nu = \sum_{i=1}^{M}\left(U_{i,\nu}c^\dagger_i + V_{i,\nu}c_i\right), \tag{2}$$

M is the dimension of the single-particle model space, which is taken to be an even integer. Coefficients U and V in the expression above define the Bogoliubov transformation. HFB state $|\phi\rangle$ is also obtained through the Bogoliubov transformation applied to the bare-particle vacuum $|0\rangle$, hence $|\phi\rangle$ corresponds to the vacuum for the quasi-particles, or $a_\nu|\phi\rangle = 0$. Indices $\nu_1,\ldots,\nu_n$ and $\nu'_1,\ldots,\nu'_{n'}$, attached to the creation and annihilation operators,

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specify quantum states in the quasi-particle basis. The symbol $[\theta]$ stands for a unitary operator

$$[\theta] \equiv \frac{e^{-i\theta\hat{S}}}{\langle\phi|e^{-i\theta\hat{S}}|\phi\rangle}, \tag{3}$$

where $\hat{S}$ is a one-body operator expressed in the quasi-particle basis [13], and θ is a parameter to specify an element in a group produced by the generator $\hat{S}$. Symbol $[\theta]$ for unitary operators is indebted to Ref. [2].

As explained in Ref. [2], such matrix elements of unitary operators shown in Eq. (1) are essential ingredients in the beyond-mean-field theories, such as quantum-number projection. In the case of angular momentum projection, the parameter θ corresponds to the Euler angles and $\hat{S}$ to the angular momentum operator $\hat{J}$.

In order to derive a formula for this matrix element Eq. (1), we will apply the Fermion coherent state and Grassmann integral. As elucidated in previous studies, these two mathematical entities show a close affinity with the Pfaffian, and they can simplify calculations involving many anti-commuting operators to a great extent. It should be noted here that Hara and Iwasaki previously investigated the mathematical structure of the matrix elements Eq. (1) [2], in connection to the Projected Shell Model (PSM) [14]. PSM is basically a configuration mixing method with multi quasi-particle states based on the HFB theory. In PSM, configuration mixing is carried out with quantum-number projected HFB states of multiple quasi-particle excitations. Hara and Iwasaki derived a formula for the matrix elements Eq. (1) with the help of a theorem presented by Balian and Brézin [15]. However, their formula suffers from the problem of combinatorial complexity, originating from the generalized Wick's theorem. According to the theorem, the matrix elements Eq. (1) involving n and n' quasi-particle excitations contain $(n+n'-1)!!$ terms. In practice, the number of terms becomes so large that it is difficult to write down matrix elements explicitly with the Hara–Iwasaki formula for more than four quasi-particle HFB states.

2. The Balian–Brézin decomposition

Following Ref. [15], a unitary operator $[\theta]$ in Eq. (3) can be expressed as a product of three operators in the quasi-particle basis,

$$[\theta] = e^{\hat{B}(\theta)} e^{\hat{C}(\theta)} e^{\hat{A}(\theta)}, \tag{4}$$

with

$$\hat{A}(\theta) = \sum_{\nu,\nu'} \frac{1}{2} A(\theta)_{\nu',\nu} a_\nu a_{\nu'},$$

$$\hat{B}(\theta) = \sum_{\nu,\nu'} \frac{1}{2} B(\theta)_{\nu',\nu} a^\dagger_\nu a^\dagger_{\nu'},$$

$$\hat{C}(\theta) = \sum_{\nu,\nu'} \big(\ln C(\theta)\big)_{\nu,\nu'} a^\dagger_\nu a_{\nu'}. \tag{5}$$

We call Eq. (4) the Balian–Brézin decomposition. Matrices $A(\theta)$, $B(\theta)$ and $C(\theta)$ in Eq. (5) correspond to contractions and can be written with the help of the Bogoliubov transformation matrices [2]

$$A_{\nu,\nu'}(\theta) \equiv \big\langle [\theta] a^\dagger_\nu a^\dagger_{\nu'} \big\rangle = \big(V^*(\theta) U^{-1}(\theta)\big)_{\nu,\nu'},$$

$$B_{\nu,\nu'}(\theta) \equiv \big\langle a_\nu a_{\nu'} [\theta] \big\rangle = \big(U^{-1}(\theta) V(\theta)\big)_{\nu,\nu'},$$

$$C_{\nu,\nu'}(\theta) \equiv \big\langle a_\nu [\theta] a^\dagger_{\nu'} \big\rangle = \big(U^{-1}(\theta)\big)_{\nu,\nu'}. \tag{6}$$

By inserting Eq. (4) into the matrix elements Eq. (1), we have

$$\mathscr{M}_I = \langle\phi| a_{\nu'_1} \cdots a_{\nu'_{n'}} e^{\hat{B}(\theta)} e^{\hat{C}(\theta)} e^{\hat{A}(\theta)} a^\dagger_{\nu_1} \cdots a^\dagger_{\nu_n} |\phi\rangle. \tag{7}$$

Hereafter, we omit symbol (θ) for the sake of brevity. For subsequent conveniences, we introduce a shorthand notation J for the indices of quasi-particle operators, as $J = \{\nu_1 \cdots \nu_n\}$, $J' = \{\nu'_1 \cdots \nu'_{n'}\}$ ($\nu_1 < \cdots < \nu_n$ and $\nu'_1 < \cdots < \nu'_{n'}$). These indices J and J' are subsets of a set $[M] = \{1, 2, \ldots, M\}$, in which M represents the number of elements in $[M]$ and corresponds to the dimension of the single-particle model space. Index I in Eq. (7) is defined as a set $I = \{\nu'_1 \cdots \nu'_{n'}, \nu_1 + M \cdots \nu_n + M\}$ and corresponds to a subset of $[2M] = \{1, 2, \ldots, 2M\}$. With these notations, the matrix elements Eq. (7) are expressed as

$$\mathscr{M}_I = \langle\phi| (a \cdots a)_{\overrightarrow{J'}} e^{\hat{B}} e^{\hat{C}} e^{\hat{A}} \big(a^\dagger \cdots a^\dagger\big)_{\overrightarrow{J}} |\phi\rangle \tag{8}$$

where $(a \cdots a)_{\overrightarrow{J'}}$ and $(a^\dagger \cdots a^\dagger)_{\overrightarrow{J}}$ stand for $a_{\nu'_1} \cdots a_{\nu'_{n'}}$ and $a^\dagger_{\nu_1} \cdots a^\dagger_{\nu_n}$, respectively.

When the order of a product is completely reversed, such an order is denoted as $\overleftarrow{J}$. The relation between $\overleftarrow{J}$ and $\overrightarrow{J}$ is given as

$$(a \cdots a)_{\overrightarrow{J}} = (a \cdots a)_{\overleftarrow{J}} (-)^{\frac{1}{2}n(n-1)}, \tag{9}$$

where $(a \cdots a)_{\overleftarrow{J}} = a_{\nu_n} \cdots a_{\nu_1}$. Note that an additional phase emerges in the right-hand side of the above equation due to anti-commutation.

3. Fermion coherent state and Grassmann integral

In the present Letter, we exclusively rely on Grassmann numbers ξ^* and ξ. They satisfy the anti-commutation rules,

$$\xi_\nu \xi_{\nu'} + \xi_{\nu'} \xi_\nu = 0, \tag{10}$$

$$\xi^*_\nu \xi^*_{\nu'} + \xi^*_{\nu'} \xi^*_\nu = 0, \tag{11}$$

$$\xi_\nu \xi^*_{\nu'} + \xi^*_{\nu'} \xi_\nu = 0, \tag{12}$$

where indices ν, ν' run from 1 to M $(1, \ldots, M)$. With these Grassmann numbers, Fermion coherent states [7] in the quasi-particle basis are defined as

$$|\boldsymbol{\xi}\rangle = e^{-\sum_\nu \xi_\nu a^\dagger_\nu} |\phi\rangle, \tag{13}$$

where the HFB state is normalized $\langle\phi|\phi\rangle = 1$. This definition is slightly different from the one introduced in Ref. [9], where the operator and the vacuum are replaced as $c_i \to a_\nu$ and $|0\rangle \to |\phi\rangle$, respectively. By definition, Fermion coherent states are eigenstates of the annihilation operator,

$$a_\nu |\boldsymbol{\xi}\rangle = \xi_\nu |\boldsymbol{\xi}\rangle. \tag{14}$$

The adjoint variable ξ^*_i is also introduced in the eigenvalue equation,

$$\langle\boldsymbol{\xi}| a^\dagger_\nu = \langle\boldsymbol{\xi}| \xi^*_\nu. \tag{15}$$

The overlap between the HFB vacuum and the Fermion coherent state is $\langle\phi|\xi\rangle = 1$. The closure relation [7] is expressed as

$$\int \mathscr{D}(\xi^*, \xi) e^{-\Sigma_\nu \xi^*_\nu \xi_\nu} |\boldsymbol{\xi}\rangle\langle\boldsymbol{\xi}| = 1, \tag{16}$$

where $\mathscr{D}(\xi^*, \xi) = \prod_\alpha d\xi^*_\alpha d\xi_\alpha$. Differential elements $d\xi$ and $d\xi^*$ are anti-commuting. Although this ordering for $\mathscr{D}(\xi^*, \xi)$ given in the above closure relation is widely employed, we use other ordering for the differential elements in the present study, which is

$$\mathscr{D}(\xi^*, \xi) = d\xi^*_{\overrightarrow{[M]}} d\xi_{\overleftarrow{[M]}} = d\xi_{\overleftarrow{[M]}} d\xi^*_{\overrightarrow{[M]}}, \tag{17}$$